

Resizing and Resolution

Working with spheres: Extra options are available when using spheres to display species. Users can resize all spheres or resize by species type, and increase the resolution for all spheres displayed before capturing images.

The radii of all spheres and cylinders drawn within the program can be adjusted in real-time. The user can alter the size of all species together, or each species independently by using the aforementioned selection method.

In tiles operation mode, when the user chooses to display crystals as “Type Spheres” (i.e. spheres coloured by tile type with the sphere radius equal to the root mean square of the tile’s coordinates) they can use the CTRL + PLUS or CTRL + MINUS keys to enlarge or shrink all sphere radii simultaneously (Figure 10, Top). By selecting a specific type with the SPACE key and using the same keyboard controls, this only affects the sphere radius of the currently selected species type (Figure 10, Centre). Users can also adjust the sphere size for each species independently when using average spheres modes.

In net spheres mode, the same options are available. Net atoms and bonds mode allows the user additional control over the display sizes of species. By selecting atoms and bonds colouring mode, each atom type is saved as a separate display list allowing each type to be resized independently. This is achieved with the same method used for tile crystals: SPACE to cycle through selected atom types and CTRL + PLUS / MINUS to adjust their sphere radii. The user can also cycle through different bond types with SHIFT + SPACE and control their cylinder radii with the same keys used for sphere radii. Varying the relative sizes of atoms is useful for studying ionic structures or for granting the user more control over the overall look of their exported images.

Additionally, users can also alter the display resolution of their spheres and cylinders. Spheres and cylinders are all constructed from strips and fans of triangles all linked together and set at different angles to give the illusion of a smooth, rounded surface. By increasing the number of triangles used to approximate a surface (i.e. splitting triangles into smaller triangles) the surface becomes smoother.

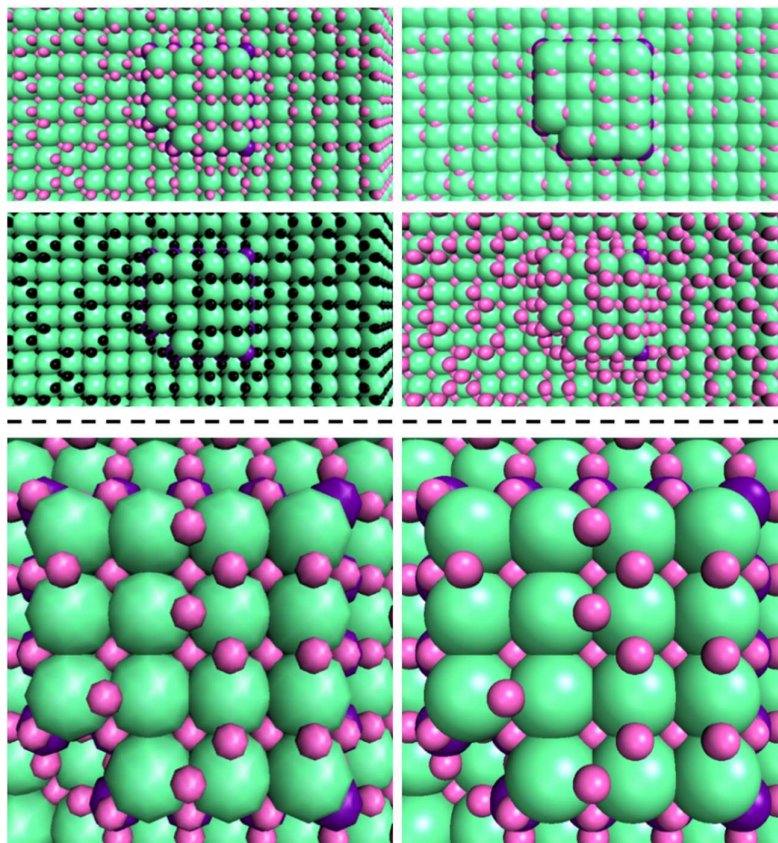


Figure 10: Images of an LTA crystal in the “type spheres” display mode. **Top Left:** With default sphere sizes. **Top Right:** With all spheres enlarged. **Centre Left:** With a single tile type selected (D4R). **Centre Right:** With the D4R spheres enlarged but all other spheres left at the default sizes. **Bottom Left:** A zoomed in image of spheres at the default low resolution to improve performance. **Bottom Right:** Spheres where the resolution has been increased for improved images, lowering performance.

To control this within the program, clicking the “Drawing” dropdown menu and selecting “Change Sphere Resolution” switches the program to allow resolution changes. This disables the “Change Sphere Size” mode. The controls for changing sphere or cylinder radii will now control the resolution of all spheres and cylinders visualised within the program (CTRL + PLUS / MINUS). By default, the resolution is set rather low (8 x 8 triangles) to increase the rendering speed while manipulating simulated crystals but can be increased before an image is taken to produce higher quality figures (Figure 10, Bottom).